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On Ex Situ NMR: Developing portable low-cost and/or single sided NMR/MRI

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Annual SEGRF report from Vasiliki Demas
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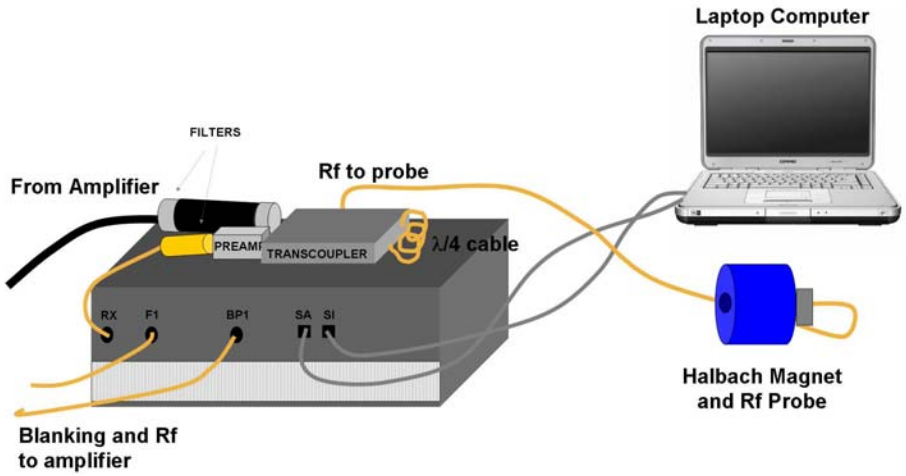
Section I -- Progress in last 12 months (May 1, 2005 - Apr 30, 2006)

Introduction to the Project

Nuclear magnetic resonance spectroscopy (NMR) is of unsurpassed versatility in its ability to non-destructively probe for chemical identity. Portable, low-cost NMR sensors would enable on site identification of potentially hazardous substances, such as signatures from production of nuclear, chemical, and biological weapon agents, narcotics, explosives, toxins, and poisons. There exist however problems that need to be considered in the case of such sensors: (a) small-scale magnets produce inhomogeneous magnetic fields and therefore undesired Larmor frequency distributions that conceal much of the useful spectral information, and (b) sensitivity in most experiments decreases due to the inherently low and strongly inhomogeneous fields associated with portable instruments. Our approach is to: (a) try to improve the field of low cost magnets either with hardware (e.g. magnet design and construction of “shim coils”) or via special pulse sequences, where the field is “effectively shimmed” to appear homogeneous to the sample, and (b) to use microcoils to improve sensitivity and to allow focusing in smaller regions and therefore smaller static field variations.

We have been working in setting up a table top, 2-Tesla permanent Halbach magnet system for tabletop NMR. The Spectrometer console is a Tecmag Apollo, controlled by a dell notebook. Currently an external linear chemagnetics rf amplifier is being used, though the power requirements for our system are quite low (a few Watts).



The Magnetic Resonance lab in LLNL, has developed several types and sizes of microcoils, which have been proven to perform well for NMR experiments. We

have evaluated an rf, 360 µm O.D., microcoil probe that was built previously. We have finished mapping the magnetic field of the magnet. In the optimal position (in terms of field quality), the field inhomogeneity was at 17ppm. Preliminary fluorine spectra with a resolved two peak separation have now been obtained. For the field, as mapped, we have initial designs of first degree shimming, or gradient coils (linear correction to the field). We have calculated "shim pulses" to effectively shim the mapped field, for ideal gradient coils. These calculations will be repeated after the coils will be built and evaluated.

Talks/Conferences
-"Progress on Ex Situ NMR" poster presentation in the 4th Alpine Conference on Solid State NMR, Chamonix (September 2005), Poster Presentation
-"Progress on Ex Situ NMR" oral presentation in the 5th Colloquium on Mobile NMR, Perugia (September 2005)
-"Ex Situ NMR: Towards a Magnetic Resonance Tricorder", Oral Presentation
In the Chemical Engineering Colloquium at UC Berkeley, (December 2005)
-"Ex Situ NMR for Chemical Analysis," Poster Presentation for SEGRF symposium (September 2005), meeting was not attended
-"Portable, Low-cost, Ex-situ NMR with Microcoils" poster presentation in the 47th Experimental Conference in NMR, Monterey (April 2006)

How much time did you spend @ LLNL over the last 12 months?
It varied from month to month, but on average 2-3days a week.

Section II -- Research plans for the next 12 months (May 1, 2006 - Apr 30, 2007)

We are working currently on the Gradient/Shim coil design and construction. Our spectrometer will be upgraded to allow their testing. Experiments will be conducted to allow for field quality improvement. Mainly, though during the next three moths I will be working on writing my thesis

"Portable, Low-Cost NMR with Laser-Lathe Lithography produced Microcoils," paper in progress

I am not planning to attend any conferences, give a talk or present a poster between May and end of July.

How much time will you spend @ LLNL over the next 12 months?
On average, 2 days per week.

Section III -- Thesis Plans (Time-Line for plan)

What is your expected graduation date? July 31, 2006
Are you on filing fee status? No
If not, when can you go on filing fee status? Full 2006
Who is on your committee? Jeffrey Reimer (ChE), Alexander Pines (Chem), David Graves (ChE), David Wemmer (Chem)
What are your plans ie stay @ LLNL or seek outside employment? Looking into both options
Who have you talked to @ LLNL regarding employment opportunities after graduation? Robert Maxwell, Julie Herberg
Have you set up a meeting with SEGRF management to discuss post-SEGRF? No